m-Tolylacetic acid

Other names:	3-Methylphenylacetic acid
	m-Methylphenylacetic acid
	Benzeneacetic acid, 3-methyl-
Inchi:	InChI=1S/C9H10O2/c1-7-3-2-4-8(5-7)6-9(10)11/h2-5H,6H2,1H3,(H,10,11)
InchiKey:	GJMPSRSMBJLKKB-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	Cc1cccc(CC(=O)O)c1
Mol. weight [g/mol]:	150.17
CAS:	621-36-3

Physical Properties

Property code	Value	Unit	Source
gf	-138.06	kJ/mol	Joback Method
hf	-268.84	kJ/mol	Joback Method
hfus	18.41	kJ/mol	Joback Method
hvap	61.99	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.622		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	3853.09	kPa	Joback Method
tb	583.03	K	Joback Method
tc	787.21	K	Joback Method
tf	340.88	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.42	J/mol×K	583.03	Joback Method
cpg	290.68	J/mol×K	617.06	Joback Method
cpg	300.33	J/mol×K	651.09	Joback Method
cpg	309.40	J/mol×K	685.12	Joback Method
cpg	317.91	J/mol×K	719.15	Joback Method
cpg	325.89	J/mol×K	753.18	Joback Method

cpg	333.35	J/mol×K	787.21	Joback Method
dvisc	0.0045711	Pa×s	340.88	Joback Method
dvisc	0.0017423	Pa×s	381.24	Joback Method
dvisc	0.0007988	Pa×s	421.60	Joback Method
dvisc	0.0004197	Pa×s	461.95	Joback Method
dvisc	0.0002445	Pa×s	502.31	Joback Method
dvisc	0.0001544	Pa×s	542.67	Joback Method
dvisc	0.0001039	Pa×s	583.03	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	394.70	K	3.50	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C621363&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume